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Numerical Simulations of Strongly Correlated Electron Systems

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After an introduction aimed at motivating the numerical study of correlated electron systems, we concentrate on two aspects of our work. The fisrt concerns algorithmic developments, namely the so called Gaussian Monte Carlo method which has the potential of circumventing the minus sign problem occurring in simulations of correlated electron systems. We then describe an application, the phase diagram of the $SU(N)$ Hubbard Heisenberg model, which exhibits exotic and novel phases of matter.

1 Introduction

The goal of solid state physics is to explain the physical properties of numerous materials in a unified framework. For simple metals, semiconductors and a class of insulators it is fair to say that this goal has been to a large extent achieved. There is however a class of materials where $d-$ and/or $f-$ shells are partially filled whose properties are harder to explain. Here, and since the electrons are confined to narrow orbitals, the Coulomb repulsion between them turns out to play a dominant role. Such strongly interacting or correlated electrons cannot be described as embedded in a static mean-field generated by the other electrons. The effect of an electron on the others is too pronounced for each to be treated independently.

The effect of correlations on material properties is often profound, and lead to a whole zoo of exotic ordering phenomena. The competition between many different order phases make those systems very sensitive to small changes in external parameters such as temperature, pressure or band-filling. For instance correlations are at the origin of the exceptionally high transition temperature (above liquid-nitrogen temperatures) of superconductors with copper-oxygen planes. In materials called heavy fermion systems the mobile electrons at low temperature behave as if their masses were a thousand time the mass of a free electron in a simple metal. Some strongly correlated electron systems exhibit big changes in resistivity as a function of applied magnetic field; colossal magneto-resistance. Such properties render the prospect of developing applications for correlated electron systems very exciting. However the very richness in phenomena and the extreme sensitivity to microscopic details, renders the theoretical study of those materials very challenging. The difficultly lies in complexity and the understanding of the emergent collective phenomena.

Our research project is centered around numerical simulations of models of correlated electron systems. The first question which one will have to address is the very choice of the model. The effect of correlations shows up at low temperatures and low energy scale. Hence, one first needs to derive effective models which describe the low temperature physical properties of the material under consideration. To this aim, one can use methods

such as the contractor-renormalization-group (CORE) method. Starting from a high energy model, the CORE essentially successively integrates out high energy degrees of freedom and produces a hierarchy of model Hamiltonians. At each iteration the model Hamiltonian is restricted to lower and lower energy or longer length scales. Hence the method acts like a magnifying glass. For example a CORE iteration will map the Hubbard model on the so-called $t - J$ model.

The second step is to solve numerically the effective low energy model. Given the complexity of the models at hand, the numerical approach is attractive since it is unbiased. At the onset the numerical problem scales exponentially with the size (i.e. the number of unit cells) of the the system. This scaling reflects the very dimension of the Hilbert space. Given this complexity it is adequate to use stochastic methods based on importance sampling; the Monte Carlo approach. In many non-trivial cases, the quantum Monte Carlo method can reduce the exponential scaling to a powerlaw. When this is achievable, it is fair to say that many properties of the system can be investigated in details on large enough system sizes so as to carry out size scaling and hence obtain results relevant for the thermodynamic limit.

In this article we will review briefly two research topics in which we are involved and which are centered around high performance computing.
i) In too many cases, simulations of systems of correlated electrons are plagued with the so called sign problem which inhibits the reduction from an exponential to algebraic scaling. There has recently been tremendous progress in this domain, in terms of algorithmic developments. In section 2 we will briefly review our activities in this domain.
ii) As mentioned above, a characteristic of correlated electron systems are competing phases leading to exotic ground states. Here we will review our work on the $SU(N)$ Hubbard-Heisenberg model, in which broken symmetry states (spin-dimerized, and d-density wave states) appear. Furthermore, the phase diagram shows an intriguing spin liquid state whose understanding is up to now not complete.

2 Gaussian Monte Carlo Methods: A Way to Circumvent the Minus Sign Problem?

As mentioned in the introduction, the stochastic approach to simulations of correlated electron systems is too often plagued by the so-called minus sign problem. Configurations, which we sample stochastically, occur with positive and negative signs thus canceling each other. This cancellation becomes nearly perfect in the limit of large lattices and low temperatures thus leading to exponential increase of the noise to signal ratio. Hence accurate low temperature results on large lattices are limited to a class of problems where one can show that the sign problem is absent. This includes non-frustrated one-dimensional systems[1], impurity models[2], electron-phonon models in arbitrary dimensions as described by the Holstein Hamiltonian, models with particle-hole symmetry[3] , multi-flavored models[4], etc. However, the physics of Hubbard type models away from the particle-hole symmetric point remains elusive.

It has long been known that the sign problem is representation dependent. In particular world line methods are unable to simulate the Hubbard model at the particle-hole symmetric point but auxiliary field methods can. The recent advance is based on a novel representation of the density matrix in terms of Gaussian operators[5]. In fact, the key point is the

observation that the density matrix of an arbitrary physical Hamiltonian can be expanded in a positive sum of Gaussian operators. This allows for sign free stochastic simulations for a wide class of models[6], including the Hubbard model.

Let us very briefly summarize the major ideas lying behind the Gaussian QMC (GQMC) approach. The interested reader may find details of the calculations in[6]. The expansion of the density matrix is done in a basis of Gaussian operators:

$$\hat{\Lambda}(\mathbf{n}) = \det(\mathbf{1}-\mathbf{n}) : e^{-\hat{\mathbf{c}}^\dagger \left(\mathbf{2}+\left(\mathbf{n}^T-\mathbf{1}\right)^{-1}\right)\hat{\mathbf{c}}} : \tag{1}$$

with $\mathbf{n}$ an $N_s \times N_s$ real matrix where N_s corresponds to the number of single particle states. $\hat{\mathbf{c}}^\dagger = \left(\hat{c}_1^\dagger, \cdots, \hat{c}_{N_s}^\dagger\right)$ where $\hat{c}_x^\dagger$ is the creation operator of a fermion in the single particle state x. Finally, $: \hat{A} :$ denotes the normal ordering of the operator $\hat{A}$. It is very convenient to work with Gaussian operators since they satisfy $\mathrm{Tr}\left[\hat{\Lambda}(\boldsymbol{n})\right] = 1$ and obey Wick's theorem such that

$$\mathrm{Tr}\left[\hat{\Lambda}(\mathbf{n})\hat{c}_x^\dagger \hat{c}_y\right] = \boldsymbol{n}_{x,y}, \quad \mathrm{Tr}\left[\hat{\Lambda}(\mathbf{n})\hat{c}_x^\dagger \hat{c}_y \hat{c}_w^\dagger \hat{c}_z\right] = \boldsymbol{n}_{x,y}\boldsymbol{n}_{w,z} + \boldsymbol{n}_{x,z}\left(\mathbf{1}-\boldsymbol{n}\right)_{w,z}. \tag{2}$$

Hence we can very easily compute the expectation value of an arbitrary observable. Since the Gaussian operators are a vastly overcomplete basis of the Fock space, it is possible to prove that an arbitrary physical density matrix can be expanded as a positive sum of Gaussian operators:

$$\hat{\rho}(\tau) = \sum_i P_i(\tau)\hat{\Lambda}(\mathbf{n}_i), \quad P_i \geq 0. \tag{3}$$

Clearly $\mathrm{Tr}\left[\hat{\rho}(\tau)\right] \equiv \sum_i P_i(\tau)$ grows exponentially with τ. One can account for this exponential growth by attaching a weight factor to the Gaussian operators thereby obtaining:

$$\hat{\rho}(\tau) = \int \mathrm{d}\underline{\boldsymbol{\lambda}} P(\underline{\boldsymbol{\lambda}}, \tau)\hat{\Lambda}(\underline{\boldsymbol{\lambda}}) \ \text{ with} \tag{4}$$

$$\underline{\boldsymbol{\lambda}} = (\Omega, \boldsymbol{n}), \ \ \hat{\Lambda}(\underline{\boldsymbol{\lambda}}) = \Omega\hat{\Lambda}(\boldsymbol{n}) \ \text{ and } \ \int \mathrm{d}\underline{\boldsymbol{\lambda}} P(\underline{\boldsymbol{\lambda}}, \tau) = 1.$$

The aim is now to formulate a stochastic process which samples the probability distribution, $P(\underline{\boldsymbol{\lambda}}, \tau)$ in the space of Gaussian operators. To achieve this goal, one can recast the imaginary time evolution of the density operator to a Fokker-Planck equation for the time evolution of the probability distribution. For a vast set of Hamiltonians $\hat{H}$, the Fokker-Planck equation can be shown to take the form:

$$\frac{\partial}{\partial\tau}P(\underline{\boldsymbol{\lambda}}, \tau) \ = \left[\frac{\partial}{\partial\Omega}\Omega h(\boldsymbol{n}) + \sum_{x,y}\frac{\partial}{\partial \boldsymbol{n}_{x,y}}\boldsymbol{A}_{x,y} + \frac{1}{2}\sum_{m,x,y,w,z}\frac{\partial^2}{\partial \boldsymbol{n}_{x,y}\partial \boldsymbol{n}_{w,z}}\boldsymbol{B}_{x,y}^{(m)}\boldsymbol{B}_{w,z}^{(m)}\right]P(\underline{\boldsymbol{\lambda}}, \tau)$$

where $\boldsymbol{B}^m$ and $\boldsymbol{A}$ are real $N_s \times N_s$ with functional dependence on $\boldsymbol{n}$ and $h(\boldsymbol{n}) = \mathrm{Tr}\left[\hat{\Lambda}(\boldsymbol{n})\hat{H}\right]$. Since the density matrix at $\tau = 0$ takes the value $\hat{\rho}(\tau = 0) = \hat{1}$ the initial condition for the Fokker-Planck equation reads: $P(\underline{\boldsymbol{\lambda}}, 0) = \delta\left(\underline{\boldsymbol{\lambda}} - (1, \mathbf{1/2})\right)$.

To solve the Fokker-Planck equation numerically, it is convenient to consider the associated stochastic differential equation. In the Ito formulation, it takes the form:

$$\mathrm{d}\Omega = -\Omega h(\boldsymbol{n})\mathrm{d}\tau \tag{5}$$

$$\mathrm{d}\boldsymbol{n} = -\boldsymbol{A}\mathrm{d}\tau + \sum_m \boldsymbol{B}^m \mathrm{d}W_m \tag{6}$$

with Wiener increments $\langle \mathrm{d}W_m \rangle = 0$, and $\langle \mathrm{d}W_m \mathrm{d}W_{m'} \rangle = \mathrm{d}\tau \delta_{m,m'}$. Eq. (5) describes the time evolution of walkers, $\underline{\boldsymbol{\lambda}}$, in the space of Gaussian operators. At $\tau = 0$, $\rho(\tau = 0) = 1$ such that all the Walkers are parameterized by $\underline{\boldsymbol{\lambda}} = (1, \mathbf{1/2})$. At imaginary time τ they are distributed according to $P(\underline{\boldsymbol{\lambda}}, \tau)$ so that we have access to the density matrix. In particular, any equal time observable is given by:

$$\langle \hat{O} \rangle \simeq \frac{\sum_i \mathrm{Tr}\left[\hat{\Lambda}(\underline{\boldsymbol{\lambda}}_i)\hat{O}\right]}{\sum_i \mathrm{Tr}\left[\hat{\Lambda}(\underline{\boldsymbol{\lambda}}_i)\right]} \tag{7}$$

where the sum runs over the set of walkers generated by the SDE. Since Wick's theorem applies for a single Gaussian operator the numerator of the above equation may easily be calculated.

As apparent from Eq. (5) the weight of a Walker at imaginary time τ reads :

$$\Omega(\tau) = e^{-\int_0^\tau \mathrm{d}\tau' h(\boldsymbol{n}(\tau'))}. \tag{8}$$

Since $\boldsymbol{n}$ is a real matrix, $h(\boldsymbol{n})$ is real and the weights remains positive! Hence the algorithm shows no explicit manifestation of the sign problem. However, the weights grow exponentially with imaginary time thus yielding an exponential increase in the variance. To circumvent this problem, one can adopt population control schemes used in Green function Monte-Carlo methods[7].

We have tested extensively the method for the Hubbard model. At high temperatures we find good agreement with benchmark results. However in the low temperature limit the sampling fails to produce a density matrix with the correct symmetries of the model. Understanding the origin of this problem is a central challenge since it opens the door to accurate, sign free, simulations of the doped Hubbard model. On the other hand, we can a posteriori impose the correct symmetries on the density matrix by projecting it on the symmetry sector of the ground state[6]. Using this procedure we find very good agreement with exact results for parameter ranges where known Monte Carlo methods such as the auxiliary field approach[8] fail due to the minus sign problem (See Fig. 1).

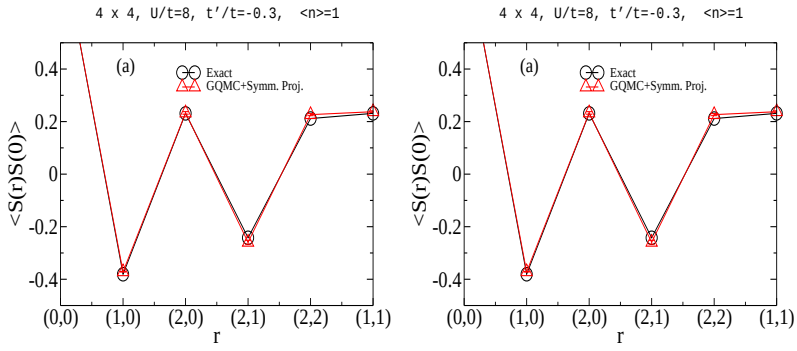

Figure 1. Real space spin-spin correlations as obtained from the GQMC and comparison with exact-diagonalization results.

3 Phase Diagram of the $SU(N)$ Hubbard-Heisenberg Model

As mentioned in the introduction, competing phases are a characteristic of systems of correlated electron systems. Here we will summarize recent numerical work on the $SU(N)$ Hubbard-Heisenberg model. Those models are relevant for the understanding of Mott insulators with orbital degeneracy as described by the Kugel-Khomskii Hamiltonian[9]. For two-fold orbital degeneracy and at a point where orbital and spin degrees of freedom play a very symmetric role, this model maps onto an $SU(4)$ symmetric Hubbard, or Heisenberg model with fundamental representation on each site[10]. On the other hand it has been argued that realizations of $SU(N)$ symmetric Hubbard models are at reach in the context of optical lattices[11].

The model we consider reads:

$$\begin{aligned} H &= H_t + H_U + H_J \quad \text{with} \\ H_t &= -t \sum_{\langle \vec{i},\vec{j} \rangle} \vec{c}^{\dagger}_{\vec{i}} \vec{c}_{\vec{j}} + \text{H.c.} \\ H_U &= \frac{U}{N} \sum_{\vec{i}} \left(\vec{c}^{\dagger}_{\vec{i}} \vec{c}_{\vec{i}} - \rho \frac{N}{2} \right) \\ H_J &= -\frac{J}{2N} \sum_{\langle \vec{i},\vec{j} \rangle} \left(D^{\dagger}_{\vec{i},\vec{j}} D_{\vec{i},\vec{j}} + D_{\vec{i},\vec{j}} D^{\dagger}_{\vec{i},\vec{j}} \right). \end{aligned} \tag{9}$$

Here, $\vec{c}^{\dagger}_{\vec{i}} = (c^{\dagger}_{\vec{i},1}, c^{\dagger}_{\vec{i},2}, \cdots, c^{\dagger}_{\vec{i},N})$ is an N-flavored spinor, $D_{\vec{i},\vec{j}} = \vec{c}^{\dagger}_{\vec{i}} \vec{c}_{\vec{j}}$ and ρ corresponds to the band-filling. In the $SU(2)$ case, the operator identity

$$\begin{aligned} \frac{-1}{4} & \left(D^{\dagger}_{\vec{i},\vec{j}} D_{\vec{i},\vec{j}} + D_{\vec{i},\vec{j}} D^{\dagger}_{\vec{i},\vec{j}} \right) = \\ & \vec{S}_{\vec{i}} \cdot \vec{S}_{\vec{j}} + \frac{1}{4} \left[(n_{\vec{i}} - 1)(n_{\vec{j}} - 1) - 1 \right] \end{aligned} \tag{10}$$

holds. Here, the fermionic representation of the spin $1/2$ operator reads $\vec{S} = \frac{1}{2} \sum_{s,s'} c^{\dagger}_{s} \vec{\sigma}_{s,s'} c_{s'}$ where $\vec{\sigma}$ are the Pauli spin matrices. Hence, at $N = 2$ the model reduces to the standard Hubbard-Heisenberg model.

In the strong coupling limit, $U/t \to \infty$, and at integer values of $\rho N/2$, charge fluctuations are suppressed. The model maps onto the $SU(N)$ Heisenberg Hamiltonian

$$H = \frac{J}{N} \sum_{\langle \vec{i},\vec{j} \rangle} \sum_{\alpha,\beta} S_{\alpha,\beta,\vec{i}} S_{\beta,\alpha,\vec{j}} \tag{11}$$

with

$$S_{\alpha,\beta,\vec{i}} = c^{\dagger}_{\alpha,\vec{i}} c_{\beta,\vec{i}} - \frac{1}{N} \delta_{\alpha,\beta} \sum_{\gamma} c^{\dagger}_{\gamma,\vec{i}} c_{\gamma,\vec{i}} \tag{12}$$

the generators of $SU(N)$ satisfying the commutation relation:

$$\left[S_{\alpha,\beta,\vec{i}}, S_{\gamma,\delta,\vec{j}} \right] = \delta_{\vec{i},\vec{j}} \left(S_{\alpha,\delta,\vec{i}} \delta_{\gamma,\beta} - S_{\gamma,\beta,\vec{i}} \delta_{\alpha,\delta} \right). \tag{13}$$

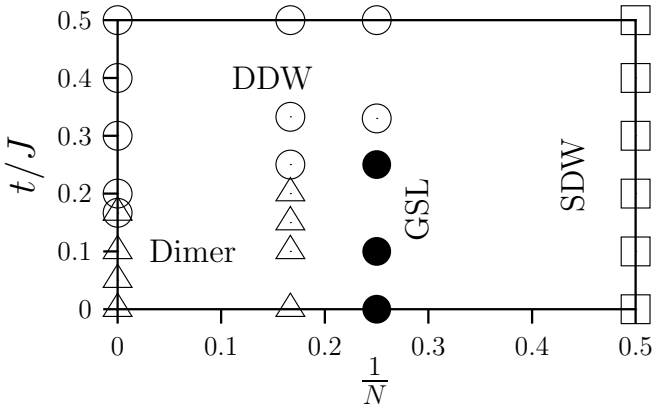

Figure 2. Phase diagram of the half-filled Hubbard-Heisenberg model as a function of t/J. Here we have set $U = 0$. The $t = 0$ line corresponds to the Heisenberg model where charge fluctuations are completely suppressed. The symbols denote the parameters where we have carried out simulations and denote the following phases: $\triangle$: Spin-dimerized phase, $\bigcirc$: DDW phase, $\square$: Spin-density wave phase, and $\bullet$: insulating phase with no broken lattice and spin symmetries and no gap spin excitations (gapless spin-liquid phase).

The representation of the $SU(N)$ group is determined by the local constraint

$$\vec{c}_{\vec{i}}^{\dagger}\vec{c}_{\vec{i}} = \rho\frac{N}{2}. \tag{14}$$

In the terminology of Young tableaux the above leads to a tableau with $\rho N/2$ rows and a single column[12]. In particular, at $N = 4$, and $\rho = 1/2$ (quarter band-filling) the model maps onto the $SU(4)$ symmetric Kugel-Khomskii Hamiltonian with fundamental representation of $SU(4)$ on each lattice site.

Our results are summarized in phase diagram of Fig. 2, and have been published in[4]. This phase diagram has attracted considerable interest, since it provides first realizations of exotic states such as the d-density wave state and the gapless spin liquid state. Let us start with the ordered phases, which are schematically shown in Fig. 3. In the spin dimerized phase, bonds joined by solid lines have a stronger exchange. This leads to an insulating spin gaped phase with broken translation symmetry. In the spin density wave phase, the spins order antiferromagnetically. Hence, translation as well as spin symmetry is broken. The DDW phase is characterized by alternating currents around elementary plaquettes. This leads to broken time and lattice symmetries. The DDW phase is a semi-metal; the single particle density of sates vanishes at the Fermi energy, but is finite at any excitation energy.

The gapless spin liquid phase (GPL) is an insulating state with algebraic staggered spin-spin correlations. It hence may be seen as a genuine Mott insulator. It's theoretical understanding is at present uncertain. A possible route one can follow to obtain a theoretical understanding is to assume that it is well described by a π-flux phase. In this case, Hermele et. al.[13] have recently argued that the SU(4) π-flux phase has a higher, $SU(8)$, emergent symmetry at low energies. The consequence of such a higher symmetry is that the asymptotic behavior of a priori very different correlation functions are locked together. For instance for our model, this higher symmetry predicts that the the $(0, \pi)$ spin-dimer

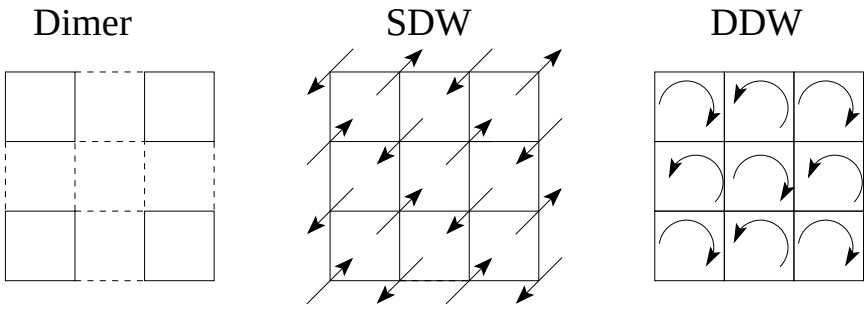

Figure 3. Schematic description of ordered phases.

correlations should have the same asymptotic behavior as the (π, π) spin-spin correlations. High accuracy large scale calculations to confirm this point of view are highly desirable.

4 Conclusions

In this article we have highlighted the complexity and interest in studies of correlated electron systems. One major challenge is on the algorithmic front. Here we are actively involved in the understanding and development of novel methods which have the potential of circumventing the so called minus sign problem for a large range of models of correlated electron systems. On the other hand, we have presented one typical application of numerical simulations of correlated electron system which leads to fascinating phase diagrams containing novel phases of matter.

Acknowledgments

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